

NUMERICAL MODELING OF AN AUTOMOTIVE DERIVATIVE PEM FUEL CELL CHP SYSTEM WITH SELECTIVE MEMBRANES

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Abstract - We present possible alternative configurations of a CHP plant based on an automotive derivative PEM fuel cell. Starting from a baseline CHP plant using the pressure swing adsorption (PSA) technology to separate hydrogen, we evaluate an alternative configuration by substituting the PSA with selective membranes.

Index Terms – CHP, Fuel Cell, Hydrogen, Membrane reactor.

I. INTRODUCTION

In the last two decades, fuel cells are entering the market of distributed CHP systems [1,2]. Specifically, PEM are the most mature and promising for commercialization [3]. Large initial costs are the major obstacle to a massive production of PEM-based CHP plants [1,2]. At the same time the EU sets the ambitious milestone of 42% global efficiency for PEM-based CHP systems.

Fuel processing, and in particular syngas purification, significantly affects both the plant cost and efficiency.

In this paper, we assess the utilization of H₂-selective membrane technology for syngas purification in comparison to traditional pressure swing adsorption (PSA).

II. DESCRIPTION OF SELECTIVE MEMBRANES

An emerging separation technology that can be an alternative to PSA-based H₂ purification, is the use of H₂-selective dense metal membranes. These membranes, based on palladium and its alloys, have frequently been proposed over the past decade to separate H₂ from a shifted syngas and simultaneously facilitate the capture of CO₂ [4]. Due to their optimum operating temperature of 300 – 500 °C, Pd-based membranes show a perfect match with the operating conditions of the WGS reaction. The H₂ flux through the membrane is driven by the difference of hydrogen partial pressure across the membrane as described by Eq. (1) [5].

$$J_{H_2} = K_{H_2} (p_{H_2,ret}^n - p_{H_2,perm}^n) \quad (1)$$

where K_{H_2} is the membrane permeance to hydrogen, $p_{H_2,ret}^n$ and $p_{H_2,perm}^n$ are the H₂ partial pressures on the retentate and permeate side of the membrane, and n is the driving force exponent.

III. POWER PLANT DESCRIPTION AND MODELING

We numerically analyze the performance of a CHP plant based on a low temperature PEM-FC. Such a plant includes a fuel processor that convert pipeline natural gas into high purity H₂, and an automotive derivative FC that produces electrical and thermal power. The baseline plant is described in details in [6]. Here, we assess the effect of substituting the PSA-based H₂ purification with selective membranes to separate H₂ from the syngas. We consider two different configurations: (i) substituting the PSA with selective membranes; (ii) integrating the membranes with the water gas shift (WGS) reactor, replacing both the WGS reactor and the PSA process. Both configurations are schematically represented in Fig. 1. The relevant processes (i.e. reforming, WGS, PSA separation membrane separation) occur at 12 bar pressure in all the configurations.

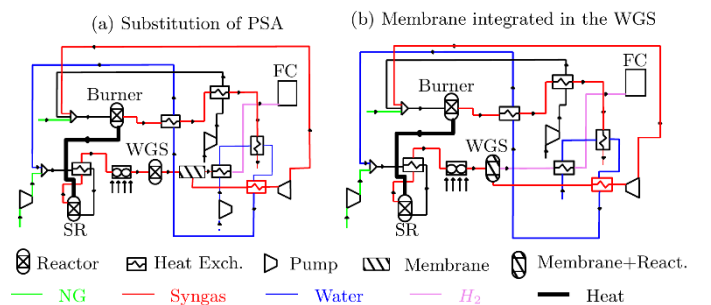


Fig. 1. Schematic representation of the considered power plants.

The steady state modelling of the power plant is performed through a thermodynamic lumped parameter approach, except for the PSA and the FC that are simulated through black-box

phenomenological models. Simulations are carried out in Aspen Plus [7] combined with proprietary Fortran models. The numerical model for the baseline plant is described in details in [6]. Following the approach in [5], the membrane reactor is modeled as a sequence of equilibrium reactors and finite area membrane separators, as represented in Fig. (2). For this, Eq. (1) is numerically integrated along the membrane surface to determine the hydrogen mass flow and concentration in the retentate and permeate gas streams.

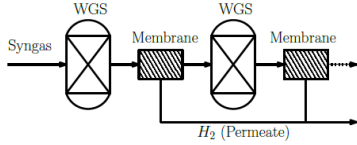


Fig. 2 Discretization of the WGS-membrane reactor.

IV. RESULTS AND DISCUSSION

We assess the effectiveness of the selective membrane integration by comparing the plant configuration presented in section II to the baseline plant described in [6] in terms of net electrical efficiency (η_{glob}) and total efficiency (η_{total}).

A. Substitution of PSA with selective membranes

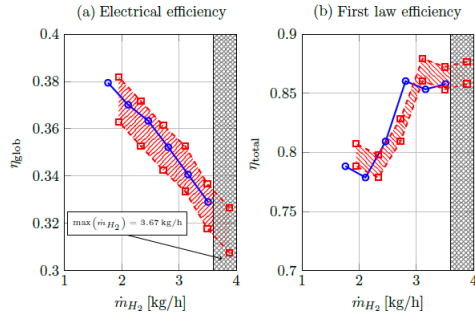


Fig. 3 Performance of the CHP plant with membrane separator after the WGS. The blue line represents the baseline plant performance. The red band between the two lines identifies the performances for atmospheric PEMFC and pressurized PEMFC (8 bar).

If H_2 is required at high pressure (i.e. 8 bar), η_{glob} is reduced (Fig. 3(a)). Such a reduction is in the range [4.4%; 5.5%]. However, if H_2 can be delivered to the FC at relatively low pressure (i.e. 1.2 bar) the membrane separator is slightly more efficient compared to the PSA. The total efficiency is not significantly varied by substituting the PSA with selective membranes.

B. Integration of selective membranes with the WGS reactor

We note from Figure 4(a) that the electrical efficiency of the modified plant is generally larger compared to the baseline configuration, except when H_2 is compressed to 8 bar. In the latter case, the power plant efficiency is only marginally reduced with respect to the baseline configuration, while for lower H_2 pressures the efficiency increment can be significant. The total efficiency is not significantly varied by substituting the PSA with the selective membranes.

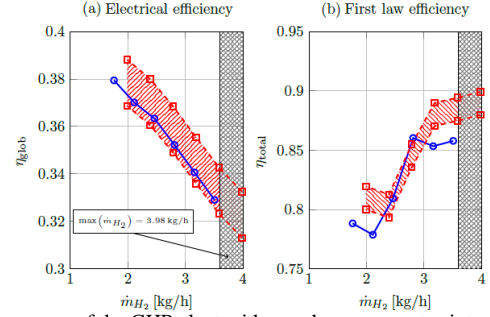


Fig. 4 Performance of the CHP plant with membrane separator integrated in the WGS. Refer to Fig. 3 for colors and symbols.

V. CONCLUSION

H_2 -selective membrane technology might improve the plant efficiency and reduce its complexity if directly integrated in the WGS. The efficiency is maximized if H_2 can be utilized at low pressure. If H_2 must be compressed the integration of selective membranes in the WGS still has a merit in terms of plant simplification. In fact, cooling and dehydration of the syngas before purification are not required.

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REFERENCES

- [1] International Energy Agency, IEA advanced fuel cells implementing agreement and annual report, 2010.
- [2] Guzy, C. PEM fuel cells for distributed generation, in Washington Fuel Cell Summit, 2012.
- [3] F. Cappa, A. L. Facci, and S. Ubertini, Proton exchange membrane fuel cell for cooperating households: A convenient combined heat and power solution for residential applications, *Energy*, Volume 90, 2015, Pages 1229-1238.
- [4] R. Bredesen, K. Jordal, O. Bolland, High-temperature membranes in power generation with CO_2 capture, *Chemical Engineering and Processing: Process Intensification*, Volume 43, 2004, Pages 1129-1158.
- [5] L. Roses, G. Manzolini, S. Campanari, E. De Wit, and M. Walter. Techno-economic assessment of membrane reactor technologies for pure hydrogen production for fuel cell vehicle fleets. *Energy & Fuels*, Volume 27, 2013, pages 4423-4431.
- [6] A. L. Facci, G. Loreti, S. Ubertini, F. Barbir, T. Chalkidis, R. P. Eßling, T. Peters, E. Skoufa, R. Bove, Numerical Assessment of an Automotive Derivative CHP Fuel Cell System, *Energy Procedia*, Volume 105, 2017, Pages 1564-1569.
- [7] Aspen Tech, Aspen Plus Unit Operation Models Reference Manual.